Molecular Spiders in One Dimension

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Molecular spiders are synthetic bio-molecular systems which have "legs" made of short single-stranded segments of DNA. Spiders move on a surface covered with single-stranded DNA segments complementary to legs. Different mappings are established between various models of spiders and simple exclusion processes. For spiders with simple gait and varying number of legs we compute the diffusion coefficient; when the hopping is biased we also compute their velocity.

I. INTRODUCTION

In recent years, chemists have constructed a number of synthetic molecular systems which can move on surfaces and tracks (see e.g. [1, 2, 3] and a comprehensive review [4]). One such object is a multi-pedal molecular spider whose legs are short single-stranded segments of DNA [5]. These spiders can move on a surface covered with single-stranded DNA segments, called substrates. The substrate DNA is complementary to the leg DNA. The motion proceeds as legs bind to the surface DNA through the Watson-Crick mechanism, then dissociate, then re-bind again, etc. More precisely, a bond on the substrate with an attached leg is first cleaved [5], and the leg then dissociates from the affected substrate (which we shall call product). The leg then rebinds again to the new substrate or to the product leading to the motion of the spider.

The rate of attachment of a leg of the spider to the substrate and the rate of detachment from the substrate are different from the corresponding rates involving the product instead of the substrate. Hence for the proper description of the motion of a single spider one must keep track of its entire trajectory. This memory requirement makes the problem non-Markovian [6, 7] and generally intractable analytically even in the case of a single spider. (We shall address this problem in a separate paper [8].) Many interacting spiders add another level of complexity. Even if the rates were the same for the substrate and the product, the properties of the spider (e.g., the nature of its gait) represent another major challenge. Here we separate this latter issue from the rest: we investigate how the structure of the spider affects its characteristics (velocity and diffusion coefficient). Further, we consider spiders with idealized gait — the goal is not to mimic complicated (and poorly known) gait of molecular spiders but to show that spiders' macroscopic characteristics are very sensitive to their structure and gait.

We shall mostly focus on a single spider moving on a lattice. We shall also assume that the rate of attachment greatly exceeds the rate of detachment. In this situation the relative time when one leg is detached is negligible and hence the possibility that two or more legs are detached simultaneously can be disregarded. Therefore the present model posits that spiders remain fully attached and never leave the surface [9]. (This differs from the actual situation when a few legs may be simultaneously detached.)

The spiders are defined as follows. Legs can jump independently at constant rates if they do not violate the restrictions below. We mainly consider symmetric spiders where we set all these rates to one, or biased spiders whose legs can only move to the right at rate one, but some special gaits are also investigated. The fundamental restriction on the spider's motion is the exclusion principle: Two legs cannot bind to the same site. Additional constraints keep the legs close to each other. We mainly consider two types of spiders with the simplest feasible constraints:

Centipedes (or local spiders). A leg of a centipede can step to nearest neighbor sites provided that it remains within distance s from the *adjacent* legs. (This threshold is assumed to be the same for each pair of adjacent legs.)

Spiders (or global spiders). Legs of these spiders can step to nearest neighbor sites as long as *all* legs remain within distance S.

The above properties of the gait guarantee that in *one dimension* the order of the legs never changes. The above constraints seem equally natural in one dimension, while in two dimensions the global constraint appears more reasonable.

We shall also briefly discuss a third type of spider where the nearest neighbor restriction on the hopping is relaxed. For these *quick spiders*, legs can step *anywhere* within distance S from *all* legs. Quick spiders have been proposed and studied numerically in Ref. [10].

The above assumptions about the gait and the disregard of memory effects leave little hope for quantitative modeling, but simplicity can help to shed light on qualitative behaviors. Therefore we study in depth a single spider with aforementioned gait moving on a one-dimensional lattice, and more briefly probe the influence of the gait and many-spider effects.

The rest of this paper is organized as follows. In Sec. II, we analyze bipedal spiders (i.e., spiders with two legs). This framework provides a useful laboratory to probe various techniques. Bipedal spiders also closely resemble molecular motors [11] and the methods developed for studying molecular motors are fruitful for studying indi-

vidual spiders [12, 13]. In Sec. III we examine multi-pedal spiders (i.e., spiders with $L \geq 3$ legs). We show that the spider with local constraint and $s = 2$ is isomorphic to a simple exclusion process (SEP) on a line with $L - 1$ sites and open boundary conditions; an even simpler isomorphism exists between spiders with global constraint and the SEP on the ring. These connections allow us to extract some spider characteristics from results about the SEP. Quick spiders are briefly investigated in Sec. IV. In Sec. V we show that the behavior of many interacting spiders can also be understood, at least in the practically important situation of low spider density, via the connection with the SEP. Finally we stress limitations of our analysis and discuss possible extensions in Sec. VI.

II. BIPEDAL SPIDER

For bipedal spiders, the local and global constraints are equivalent, $s \equiv S$. For the simplest mobile bipedal spider, the allowed distance between the legs is one or two lattice spacing, i.e., $s = 2$. Two possible configurations are (up to translation)

$$\ldots \circ \bullet \bullet \circ \ldots \qquad \text{and} \qquad \ldots \circ \bullet \circ \bullet \circ \ldots \qquad (1)$$

where we denote empty sites by 'o' and filled sites (to which the legs are attached) by '•'. There are obvious back and forth transitions between these configurations:

$$\bullet \bullet \circ \Longleftrightarrow \bullet \circ \bullet \qquad \text{and} \qquad \circ \bullet \bullet \Longleftrightarrow \bullet \circ \bullet$$

For symmetric spiders each leg jumps at rate one when possible, hence all the above four elementary moves happen at rate unity. The diffusion coefficient of this bipedal spider is

$$D_2 = \frac{1}{4} \qquad (2)$$

To put this in perspective, we note that the diffusion coefficient of a random walker which hops to the right and left with unit rates is $D = 1$. Thus adding a leg and requiring the legs to stay within distance two to each other reduces the diffusion coefficient by a factor 4.

Generally for symmetric bipedal spiders with arbitrary s, there are s possible configurations $\mathcal{C}_\ell$ labeled by the inter-leg distance, $\ell = 1, \ldots, s$. The transitions are

$$\mathcal{C}_1 \Longleftrightarrow \mathcal{C}_2 \Longleftrightarrow \ldots \Longleftrightarrow \mathcal{C}_s$$

The diffusion coefficient D_s of this bipedal spider is

$$D_s = \frac{1}{2} \left(1 - \frac{1}{s} \right) \qquad (3)$$

The above results apply to symmetric bipedal spiders which hop to the left and right with equal rates. Molecular motors usually undergo directed motion [11], and one of the goals of future research is to control spiders to move preferentially in a certain direction. Here we analyze such directed motion theoretically. For concreteness, we focus on the extreme bias when each leg can only hop to right at rate one. For instance, for the bipedal spider the most compact configuration evolves via $\bullet \bullet \circ \Longrightarrow \bullet \circ \bullet$; the process $\circ \bullet \bullet \Longrightarrow \bullet \circ \bullet$ involves hopping to the left and therefore it is forbidden in the biased case.

For biased bipedal spiders the velocity and the diffusion coefficient are given by

$$V_s = 1 - \frac{1}{s} , \qquad D_s = \frac{1}{3} \left(1 - \frac{1}{s} \right) \left(1 - \frac{1}{2s} \right) \qquad (4)$$

In this section we give a pedestrian derivation of (3). The expressions (4) for velocity and diffusion coefficient can be derived by utilizing the same technique; instead, we shall extract them from more general results for lame spiders (Sec. II C).

To set the notation and to explain how we compute the diffusion coefficient we begin with a random walk (which is a one-leg spider). Let $P_n(t)$ be the probability that the random walker is at site n at time t. This quantity evolves according to

$$\frac{dP_n}{dt} = P_{n-1} + P_{n+1} - 2P_n \qquad (5)$$

One can solve this equation and then use that solution to extract the diffusion coefficient. In the case of the spiders, however, master equations generalizing (5) are much less tractable, and therefore a more direct way of computing the diffusion coefficient is preferable. Here we describe one such approach [7]. It involves two steps. First, one ought to determine the mean-square displacement

$$\langle x^2 \rangle = \sum_{n=-\infty}^{\infty} n^2 P_n \qquad (6)$$

Then the basic formula [7]

$$D = \lim_{t \to \infty} \frac{\langle x^2 \rangle}{2t} \qquad (7)$$

allows to extract the diffusion coefficient.

For the random walk, the mean-square displacement evolves according to

$$\frac{d}{dt} \langle x^2 \rangle = \sum_{n=-\infty}^{\infty} n^2 \left(P_{n-1} + P_{n+1} - 2P_n \right) \qquad (8)$$

Transforming the first two sums we obtain

$$\sum_{n=-\infty}^{\infty} n^2 P_{n \mp 1} = \sum_{n=-\infty}^{\infty} (n \pm 1)^2 P_n \qquad (9)$$

These identities allow us to recast (8) into

$$\begin{aligned} \frac{d}{dt} \langle x^2 \rangle &= \sum_{n=-\infty}^{\infty} \left[(n+1)^2 + (n-1)^2 - 2n^2 \right] P_n \\ &= 2 \sum_{n=-\infty}^{\infty} P_n = 2 \end{aligned}$$

where the last equality follows from normalization. Thus $\langle x^2 \rangle = 2t$. Plugging this into (7) we recover the diffusion coefficient of the random walker $D = 1$.

We now turn to the bipedal spider. We shall examine in detail only symmetric hopping.

A. Bipedal Spider with $s = 2$

For the bipedal spider with $s = 2$ there are two possible spider configurations. Denote by $P_n(t)$ and $Q_n(t)$ the probabilities that at time t the spider is in respective configurations (1), namely

$$P_n = \text{Prob}[\bullet\,\bullet], \quad Q_n = \text{Prob}[\bullet \circ \bullet], \qquad (10)$$

with the left leg being at site n. The governing equations for these probabilities are

$$\frac{dP_n}{dt} = Q_n + Q_{n-1} - 2P_n \qquad (11a)$$

$$\frac{dQ_n}{dt} = P_{n+1} + P_n - 2Q_n \qquad (11b)$$

The mean position of the legs or the 'center of mass' of the spider in a configuration corresponding to P_n (resp. Q_n) is located at $n + \frac{1}{2}$ (resp. $n + 1$). Thus the mean-square displacement is

$$\langle x^2 \rangle = \sum_{n=-\infty}^{\infty} \left[\left(n + \frac{1}{2} \right)^2 P_n + (n+1)^2 Q_n \right] \qquad (12)$$

and it evolves according to

$$\frac{d}{dt} \langle x^2 \rangle = \sum_{n=-\infty}^{\infty} \left(n + \frac{1}{2} \right)^2 (Q_n + Q_{n-1} - 2P_n)$$
$$+ \sum_{n=-\infty}^{\infty} (n+1)^2 (P_{n+1} + P_n - 2Q_n)$$

Utilizing the same tricks as in (9) we recast the above equation into

$$\frac{d}{dt} \langle x^2 \rangle = \frac{1}{2} \sum_{n=-\infty}^{\infty} (P_n + Q_n) = \frac{1}{2} \qquad (13)$$

The last identity is implied by normalization and its validity also follows from Eqs. (11a)–(11b). Integrating (13) yields $\langle x^2 \rangle = \frac{1}{2} t$ which in conjunction with (7) leads to the previously announced result, Eq. (2).

B. General Case

In the general case ($s \geq 2$) we denote

$$P_n^\ell = \text{Prob}[\bullet \underbrace{\circ \cdots \circ}_{\ell-1} \bullet] \qquad (14)$$

the probability to occupy sites n and $n + \ell$. These probabilities obey

$$\frac{dP_n^1}{dt} = P_{n-1}^2 + P_n^2 - 2P_n^1 \qquad (15a)$$

$$\frac{dP_n^\ell}{dt} = P_{n-1}^{\ell+1} + P_{n+1}^{\ell-1} + P_n^{\ell+1} + P_n^{\ell-1} - 4P_n^\ell \qquad (15b)$$

$$\frac{dP_n^s}{dt} = P_{n+1}^{s-1} + P_n^{s-1} - 2P_n^s \qquad (15c)$$

where equations (15b) apply for $2 \leq \ell \leq s - 1$. The mean-square displacement is given by

$$\langle x^2 \rangle = \sum_{n=-\infty}^{\infty} \sum_{\ell=1}^{s} \left(n + \frac{\ell}{2} \right)^2 P_n^\ell \qquad (16)$$

Using Eqs. (15a)–(15c) and applying the same tricks as above to simplify the sums, we obtain

$$\frac{d}{dt} \langle x^2 \rangle = \sum_{\ell=1}^{s} w_\ell - \frac{1}{2} (w_1 + w_s) \qquad (17)$$

where $w_\ell = \sum_n P_n^\ell$ is the weight of configurations of the type $\mathcal{C}_\ell$. The sum on the right-hand side of Eq. (17) is equal to one due to normalization. To determine w_1 and w_s one does not need to solve an infinite set of the master equations (15a)–(15c). Instead, we take Eqs. (15a)–(15c) and sum each of them over all n to yield a closed system of equations for the weights

$$\frac{dw_1}{dt} = 2(w_2 - w_1) \qquad (18a)$$

$$\frac{dw_\ell}{dt} = 2(w_{\ell-1} + w_{\ell+1} - 2w_\ell) \qquad (18b)$$

$$\frac{dw_s}{dt} = 2(w_{s-1} - w_s) \qquad (18c)$$

If initially $w_1 = \ldots = w_s = 1/s$, then Eqs. (18a)–(18c) show that this remains valid forever. Even if we start with an arbitrary initial condition, all the weights w_s relax exponentially fast toward the 'equilibrium' value $1/s$. Thus the right-hand side of (17) becomes $1 - 1/s$ yielding $\langle x^2 \rangle = (1 - 1/s)\,t$ which in conjunction with (7) leads to Eq. (3).

C. Heterogeneous Spiders

Various spiders can be assembled experimentally [5], including those with distinguishable legs. Here we analyze the coarse-grained properties of these 'lame' spiders.

The bipedal lame spider is characterized by the maximal separation s between the legs and by the hopping rates α and β of the legs, e.g., the α-leg hops to the right and left with the same rate α (whenever hopping is possible) in the symmetric case. For the bipedal spider with $s = 2$, the diffusion coefficient is given by

$$D_2 = \frac{1}{2} \frac{\alpha\beta}{\alpha + \beta} \qquad (19)$$

When $\alpha = \beta$ we recover the already known result telling us that the diffusion coefficient is 4 times smaller than the hopping rate. For a very lame spider ($\alpha \ll \beta$), Eq. (19) gives $D_2 = \alpha/2$, so the diffusion coefficient is half the hopping rate of the very slow leg.

To derive (19), we first note that the probabilities (10) satisfy

$$\frac{dP_n}{dt} = \beta Q_n + \alpha Q_{n-1} - (\alpha + \beta)P_n \qquad (20a)$$

$$\frac{dQ_n}{dt} = \alpha P_{n+1} + \beta P_n - (\alpha + \beta)Q_n \qquad (20b)$$

Here we have assumed that the left leg hops with rate α and the right leg hops with rate β. (Recall that in one dimension, the order of the legs never changes.)

Using Eqs. (20a)–(20b) we find that the mean-square displacement (13) evolves according to

$$\frac{d}{dt}\langle x^2 \rangle = \frac{\alpha + \beta}{4} - (\alpha - \beta)(u - v) \qquad (21)$$

where

$$u = \sum_{n=-\infty}^{\infty} \left(n + \frac{1}{2}\right) P_n, \quad v = \sum_{n=-\infty}^{\infty} (n+1)Q_n$$

From Eqs. (20a)–(20b) we deduce that the quantity $u - v$ obeys

$$\frac{d}{dt}(u - v) = \frac{\alpha - \beta}{2} - 2(\alpha + \beta)(u - v) \qquad (22)$$

Equation (22) shows that $u - v$ quickly approaches to $(\alpha - \beta)/[4(\alpha + \beta)]$. Plugging this into (21) yields

$$\frac{\langle x^2 \rangle}{t} \to \frac{1}{4}\left[\alpha + \beta - \frac{(\alpha - \beta)^2}{\alpha + \beta}\right] = \frac{\alpha\beta}{\alpha + \beta}$$

which leads to the announced result, Eq. (19).

For the biased bipedal lame spider, the drift velocity is given by a neat formula

$$V_2 = \frac{\alpha\beta}{\alpha + \beta} \qquad (23)$$

which resembles to (19). To establish (23) one can use the analog of Eqs. (20a)–(20a), namely

$$\frac{dP_n}{dt} = \alpha Q_{n-1} - \beta P_n \qquad (24a)$$

$$\frac{dQ_n}{dt} = \beta P_n - \alpha Q_n \qquad (24b)$$

Equations (24a)–(24b) give the weights

$$w_1 \equiv \sum_{n=-\infty}^{\infty} P_n = \frac{\alpha}{\alpha + \beta}, \quad w_2 \equiv \sum_{n=-\infty}^{\infty} Q_n = \frac{\beta}{\alpha + \beta}$$

and relation $V = (\beta w_1 + \alpha w_2)/2$ leads to (23).

Further analysis of Eqs. (24a)–(24b) allows one to determine the diffusion coefficient

$$D_2 = \frac{1}{2}\alpha\beta \frac{\alpha^2 + \beta^2}{(\alpha + \beta)^3} \qquad (25)$$

We do not give a derivation of this formula since it can be extracted from earlier results by Fisher and Kolomeisky [12] who in turn used previous findings by Derrida [13].

It is more difficult to compute the diffusion coefficient for the bipedal lame spider with maximal span $s > 2$. The results of Ref. [12] do not cover the general case, although a proper extension of methods [12, 13] may solve the problem. For the symmetric bipedal lame spider with maximal span $s \geq 2$, we used an approach outlined in Appendix A and obtained

$$D_s = \frac{\alpha\beta}{\alpha + \beta}\left(1 - \frac{1}{s}\right). \qquad (26)$$

For $s = 2$, we recover equation (19).

For the biased bipedal lame spider with maximal span $s \geq 2$ it is again simple to determine the drift velocity. Using an analog of (24a)–(24b) one gets the weights and then the drift velocity is found from the relation

$$2V_s = \beta w_1 + (\alpha + \beta)\sum_{\ell=2}^{s-1} w_\ell + \alpha w_s$$

The outcome of this computation is

$$V_s = \alpha\beta \frac{\alpha^{s-1} - \beta^{s-1}}{\alpha^s - \beta^s} \qquad (27)$$

Specializing to $\alpha = \beta = 1$ (the l'Hospital rule allows to resolve an apparent singularity) one arrives at the expression (4) for the velocity.

Finally, the diffusion coefficient for the biased bipedal spider with arbitrary s is

$$\begin{aligned} D_s =\ & \frac{1}{2}\alpha\beta \frac{\alpha^{s-1} - \beta^{s-1}}{\alpha^s - \beta^s} \\ & + \frac{1+s}{\alpha^s - \beta^s}\frac{\alpha^{s-1} - \beta^{s-1}}{\alpha^s - \beta^s}\frac{\alpha^{s+1}\beta^{s+1}}{\alpha^s - \beta^s} \\ & + \frac{1-s}{\alpha^s - \beta^s}\frac{\alpha^{s+1} - \beta^{s+1}}{\alpha^s - \beta^s}\frac{\alpha^s\beta^s}{\alpha^s - \beta^s}. \end{aligned} \qquad (28)$$

This equation is derived in Appendix A.

Equation (28) reduces to (25) when $s = 2$; for $s = 3$, the diffusion coefficient can be re-written as

$$D_3 = \frac{1}{2}\alpha\beta \frac{(\alpha + \beta)(\alpha^2 - \alpha\beta + \beta^2)(\alpha^2 + 3\alpha\beta + \beta^2)}{(\alpha^2 + \alpha\beta + \beta^2)^3}$$

Also when $\alpha = \beta = 1$, equation (28) reduces to the expression (4) for the diffusion coefficient.

III. MULTI-PEDAL SPIDERS

For the multi-pedal spider, $L \geq 3$, we must specify the constraint governing the separations between the legs.
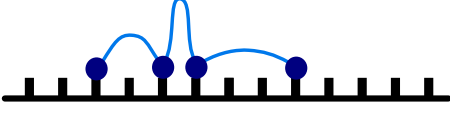
FIG. 1: Illustration of a centipede, i.e. a spider with local constraint. All legs step to empty nearest neighbor sites at the same rate with adjacent legs staying within distance s from each other.

A. Centipedes

Here we consider centipedes or local spiders where the distance between the jth and $(j+1)^{\text{st}}$ legs is at most s. See Fig. 1 for an illustration of such a centipede. In this case the total number of configurations is $\mathcal{C} = s^{L-1}$ since each of the $(L-1)$ spacings between adjacent legs can have s possible values.

1. Main results

Consider first spiders with $s = 2$. The configurations for the bipedal spider are shown in (1); the four possible configurations for the tripod are

$$\bullet\bullet\bullet \qquad \bullet\circ\bullet\bullet \qquad \bullet\bullet\circ\bullet \qquad \bullet\circ\bullet\circ\bullet \qquad (29)$$

and generally there are 2^{L-1} possible configurations.

Let $D(L)$ be the diffusion coefficient of an L-leg spider. In the case of symmetric hopping (all rates are one)

$$D(L) = \frac{1}{4(L-1)} \qquad (30)$$

when $s = 2$. For $L = 2$, this of course agrees with our previous result: $D(2) = D_2 = 1/4$.

For the biased multi-pedal spider, the velocity is

$$V(L) = \frac{1}{2}\frac{L+1}{2L-1} \qquad (31)$$

The biased infinite-leg spider has a finite limiting speed! More precisely, $V(\infty) = 1/4$, i.e., the infinite-leg spider drifts 4 times slower than the single-leg spider. The diffusion coefficient of the biased spider is

$$D(L) = \frac{3}{4}\frac{(4L-3)!\,[(L-1)!(L+1)!]^2}{[(2L-1)!]^3\,(2L+1)!} \qquad (32)$$

Note that the diffusion coefficient of the infinite-leg spider vanishes. Asymptotically,

$$D(L) \sim \frac{3\sqrt{2\pi}}{128}\,L^{-1/2} \quad \text{as} \quad L \to \infty \qquad (33)$$

The above results (30)–(32) are valid when $s = 2$. We have not succeeded in computing $V(L)$ and $D(L)$ for arbitrary L when the maximal separation exceeds two, $s > 2$.

The velocity and the diffusion coefficient can be computed for centipedes with $s > 2$ when the number of legs

is sufficiently small. The simplest quantity is the velocity of biased spiders. When $s = 3$, we computed the velocity $V(L)$ of centipedes with up to seven legs:

$$V(2) = 2/3$$
$$V(3) = 26/45 \approx 0.5778$$
$$V(4) = 2306/4301 \approx 0.5362$$
$$V(5) = \frac{2257932864491452}{4410656468591479} \approx 0.5119$$
$$V(6) \approx 0.4960476429$$
$$V(7) \approx 0.4848259795$$

(we have not displayed exact expressions for $V(6)$ and $V(7)$ which are the ratios of huge integers.) Note that for biased spiders with $s = 3$ one can guess the general expression (31) from exact results for $V(L)$ for small L; in contrast, no simple expression seems to exist for the velocity of biased spiders with $s > 2$.

For symmetrically hopping spiders, we computed the diffusion coefficient when the number of legs is small. Here are the results for centipedes with $s = 3$ (the method used in calculations is described in Appendix A)

$$D(2) = 1/3$$
$$D(3) = 22/117 \approx 0.1880$$
$$D(4) = 530/4059 \approx 0.1306$$
$$D(5) = \frac{145730406362990}{1457669284934841} \approx 0.0999749$$
$$D(6) = \frac{13157424169190800305558220463956878370565}{162454344889141072641777603974162004103911}$$
$$\approx 0.080991519$$

In contrast to the neat formula (30) characterizing the $s = 2$ case, the above numbers look intimidating. Factorizing the nominator and denominator of $D(6)$ reveals the presence of extraordinary huge factors and thereby excludes that it can be described by a formula like (32), let alone (30). Note that at least the L^{-1} asymptotic behavior predicted by Eq. (30) remains valid for all s; for $s = 3$, in particular, we have $D(L) \sim AL^{-1}$ with $A \approx 0.423$ when $L \gg 1$.

2. Mapping to the exclusion process for $s = 2$

The derivations of above results are complicated since the number of configurations grows exponentially with L. Further, the transition rates are configuration dependent, e.g., for the four-leg spider configurations

$$\bullet\bullet\bullet\bullet \qquad \bullet\circ\bullet\bullet\bullet \qquad \bullet\bullet\circ\bullet\bullet$$

evolve with rates 2, 3, 4 for symmetric hopping. (In contrast, for bipedal spiders the number of configurations grows linearly with s and the transition rates are simple.) All this makes the computation of the diffusion coefficient $D(L)$ for arbitrary L very challenging. The pedestrian

calculation is feasible for small L, but even for $L = 3$, the framework based on rate equations like (15a)–(15c) is very cumbersome.

Fortunately, spiders with local constraint and $s = 2$ are related to simple exclusion processes (SEPs). This allows us to extract some predictions about spiders from previously known results about SEPs, and to employ the methods developed in the context of SEPs to situations natural in applications to spiders.

We now demonstrate the remarkable connection between centipedes with $s = 2$ and SEPs. As an example we show that the biased spider is isomorphic to the totally asymmetric simple exclusion process (TASEP) with open boundary conditions. To understand the isomorphism, consider for concreteness the tripod. We can map configurations (29) onto configurations

$$00 \qquad 10 \qquad 01 \qquad 11 \qquad (34)$$

of the exclusion process on two sites with open boundary conditions. Here 0 on j^{th} site implies that there is no empty site between j^{th} and $(j+1)^{\text{st}}$ legs, while 1 implies that there is an empty site. A hop to the right of an internal leg in (29) corresponds to a hop to the left of a particle in (34). Further, the hop of an extreme right leg corresponds to the addition of a particle to the extreme right position, and the hop of the extreme left leg corresponds to the removal of a particle from the extreme left position. The same mapping applies to any L. Thus in this TASEP each site $i = 1, \ldots, L - 1$ can be occupied by a particle, and each particle hops to the left with rate one if this site is empty; further, a particle is added to site $i = L - 1$ with rate one if this site is empty, and a particle is removed from site 1 with rate one if this site is occupied. Thus we have shown that the $s = 2$ biased spider that moves to the right is equivalent to the TASEP with open boundaries in which particles hop from right to left. A similar mapping holds between the symmetric spider and the symmetric exclusion process.

Derrida, Domany, and Mukamel [14] have shown that Eq. (31) gives the flux in the TASEP; the isomorphism between the flux and velocity proves that the velocity of the biased spiders is given by (31). This result was rederived by other techniques, e.g., by a pure combinatorial approach [15]. The (much more complicated) derivation of the diffusion coefficient in Ref. [16] gives (32).

3. Derivation of (30)

For the symmetric spider, it should be possible to compute the diffusion coefficient (30) by using the technique of Ref. [16]. This technique (based on an extension of a matrix technique) is very advanced. The final result (30) looks much simpler than its biased counterpart (32). Hence we have sought another derivation, and we have found an intriguingly simple proof of (30) based on the fluctuation-dissipation formula (see Appendix B).

First we recall that the symmetric spider with L legs hopping in both directions with rates equal to 1 is equivalent to a symmetric exclusion process on $L - 1$ sites with open boundary conditions. For this SEP, *all* rates (i.e. hopping rates in the bulk, entrance and exit rates at the boundaries) are equal to 1. This Markov process satisfies detailed balance and is at equilibrium; in particular, the mean current, i.e., the velocity of the spider, vanishes identically. The variance of the current corresponds to the diffusion constant of the spider. This variance can be calculated as follows.

Consider now a symmetric exclusion process of length $L - 1$ with open boundaries and *arbitrary* addition and removal rates at the boundaries. The system is driven out of equilibrium by particles entering and leaving at the boundaries. In the bulk, each particle hops with rates 1 to the right and to the left (if the corresponding sites are empty); a particle enters at site 1 with rate α and leaves this site with rate γ; similarly a particle enters another boundary site $L - 1$ with rate δ and leaves this site with rate β. Generically, these unequal rates lead to a current. The mean value of this current is given by (see e.g. Ref. [17])

$$J = \frac{\frac{\beta}{\beta+\delta} - \frac{\gamma}{\alpha+\gamma}}{L + \frac{1}{\alpha+\gamma} + \frac{1}{\beta+\delta} - 2} . \qquad (35)$$

The equilibrium conditions correspond to $\alpha = \gamma = \beta = \delta = 1$ and $J = 0$. We now choose the rates on site 1 as follows $\alpha = \exp(\frac{\epsilon}{2})$ and $\gamma = \exp(-\frac{\epsilon}{2})$ and we keep $\beta = \delta = 1$ at site $L - 1$. Then, the current is given by

$$J = \frac{\tanh \frac{\epsilon}{2}}{2L - 3 + \frac{1}{\cosh \frac{\epsilon}{2}}} . \qquad (36)$$

The Markov matrix of this process satisfies the generalized detailed balance condition given by equation (B2) of the Appendix B, with $y = \pm 1$ if a particle enters at site 1, or exits from site 1 ($y = 0$ otherwise). We can then use the fluctuation-dissipation formula (see (B4) in the Appendix B) wich tells us that the fluctuation of the current at the first site is given by

$$D = \left. \frac{\partial J}{\partial \epsilon} \right|_{\epsilon=0} = \frac{1}{4(L-1)} , \qquad (37)$$

in accordance with equation (30).

4. Mean-field approximation for $s \geq 3$

Simple exclusion processes have been thoroughly investigated (see books and reviews [18, 19, 20, 21]). Hence one can extract the results about spiders from already known results about SEP. Unfortunately, for spiders with local constraint the mapping onto SEP applies only when $s = 2$. The spider with L legs and arbitrary s can be mapped onto an exclusion-like process with $L - 1$ sites

and with open boundaries. In this process the maximal occupancy is limited, namely the number of particles in each site cannot exceed $s - 1$. The dynamics is simple: one chooses sites with rate one and moves a particle to the site on its left; nothing happens if the chosen site was empty or the site on the left was fully occupied. One also adds particles to site $i = L - 1$ and removes from site $i = 1$, both these processes occur with rate one; the addition is possible as long as site $i = L - 1$ is not fully occupied (contains no more than $s - 1$ particles). Unfortunately, this neat process has not been solved exactly but it can be studied by a mean-field analysis.

To simplify the analysis, we consider centipedes with infinitely many legs. We assume that the distance between adjacent legs cannot exceed s. We further assume that the spider's motion is biased, and limit ourselves to a (mean-field) computation of its velocity $V^{(s)}$.

First we map the spider onto the generalized asymmetric exclusion process with at most $s - 1$ particles per site. We then write x_j for the density of sites with j particles; this is just the density of gaps of length $j + 1$ between adjacent legs of the spider. The possible values are $j = 0, \ldots, s - 1$. Writing the evolution equation for $\dot{x}_j$ and setting $\dot{x}_j = 0$ we obtain

$$(x_{j-1} - x_j)(1 - x_0) - (x_j - x_{j+1})(1 - x_{s-1}) = 0 \quad (38)$$

when $1 \leq j \leq s - 2$. Similarly from $\dot{x}_0 = 0$ and $\dot{x}_{s-1} = 0$ we get

$$x_1(1 - x_{s-1}) - x_0(1 - x_0) = 0 \quad (39a)$$
$$x_{s-2}(1 - x_0) - x_{s-1}(1 - x_{s-1}) = 0 \quad (39b)$$

The obvious normalization requirement is

$$\sum_{j=0}^{s-1} x_j = 1 \quad (40)$$

As a warm up, consider the first non-trivial case $s = 3$. Due to normalization, it is sufficient to use (39a)–(39b). Writing $x_0 \equiv x$ and $x_2 \equiv z$, we have $x_1 = 1 - x - z$ from (40), and (39a)–(39b) become

$$(1 - x - z)(1 - z) = x(1 - x) \quad (41a)$$
$$(1 - x - z)(1 - x) = z(1 - z) \quad (41b)$$

These equations are actually identical; solving any of them we arrive at

$$x = 1 - \frac{z + \sqrt{z(4 - 3z)}}{2} \quad (42)$$

To compute velocity we return to the original formulation. A leg of the spider moves with rate 1 if the site ahead is empty and if the leg behind is one or two steps behind. The former event happens with probability $1 - x$, while the latter occurs with probability $1 - z$. Thus the velocity is

$$V^{(3)} = (1 - x)(1 - z) \quad (43)$$

Using (42) we get

$$V = \frac{1}{2}(1 - z)\left[z + \sqrt{z(4 - 3z)}\right] \quad (44)$$

We should select maximal velocity. The maximum of $V(z)$ given by (44) is reached at $z = 1/3$, and it reads

$$V^{(3)} = \frac{4}{9} \quad (45)$$

At the state corresponding to the actual (maximal) velocity all densities are equal: $x_0 = x_1 = x_2 = 1/3$.

The situation for $s > 3$ is also simple. Analyzing recurrence (38) one finds that for all $0 \leq j \leq s - 1$ the solution is a shifted geometric progression

$$x_j = A + B\lambda^j, \qquad \lambda = \frac{1 - x_0}{1 - x_{s-1}} \quad (46)$$

Plugging (46) into Eqs. (39a)–(39b) one achieves the consistency if either $A = 0$ or $\lambda = 1$. In the latter case the densities are the same, and hence they are all equal to s^{-1} due to normalization requirement (40). The straightforward generalization of (43) is

$$V^{(s)} = (1 - x_0)(1 - x_{s-1}) \quad (47)$$

and therefore

$$V^{(s)} = \left(1 - \frac{1}{s}\right)^2 \quad (48)$$

In the complimentary case of $A = 0$ the analysis is a bit more lengthy. However, the final result is the same. Here is the proof. Since $x_j = B\lambda^j$, equation (46) gives $\lambda = (1 - B)/(1 - B\lambda^{s-1})$, which can be re-written as

$$B = \frac{1 - \lambda}{1 - \lambda^s} \quad (49)$$

Further, (47) becomes

$$V^{(s)} = (1 - B)(1 - B\lambda^{s-1}) \quad (50)$$

Using (49) we recast (50) into

$$V^{(s)}(\lambda) = \lambda\left(\frac{1 - \lambda^{s-1}}{1 - \lambda^s}\right)^2 \quad (51)$$

The maximum of $V^{(s)}(\lambda)$ is achieved at $\lambda = 1$. Thus the velocity is indeed given by Eq. (48).

The above elementary analysis is mean-field as we have assumed the validity of the factorization. The answer is trivially exact for $s = 1$, and it is known to be exact for $s = 2$. For $s = 3$, we calculated velocities exactly for small centipedes, see Sect. III A 1. The limiting $L \to \infty$ value obtained from simulations $V^{(3)} \approx 0.4189$ is close to the predicted mean-field value $V^{(3)} = 4/9 \approx 0.4444$. Overall, the assumed factorization is not exact when $s \geq 3$. Note that a model which differs from our model only in the hopping rules has been solved exactly [22], but there the stationary state is a product measure.

5. Lame spiders

Finally we investigate lame centipede spiders whose extreme left leg hops to the right with rate α and the extreme right leg hops to the right with rate β. The above mean-field analysis shows that the velocity of the extreme left leg is $\alpha(1 - x_0)$ and the velocity of the extreme right leg is $\beta(1 - x_{s-1})$. As long as these velocities exceed the bulk velocity (48), the actual gap density x_0 at the left end and x_{s-1} at the right end will be higher than their bulk values, so the spider will move with velocity (48). This occurs as long as $\alpha(1 - s^{-1})$ and $\beta(1 - s^{-1})$ exceed $(1 - s^{-1})^2$, i.e. $\alpha, \beta \geq 1 - s^{-1}$. When at least one of the rates is smaller than the threshold value, different behaviors emerge. Overall, the speed of the infinite-leg spider exhibits an amusing dependence on the rates α and β:

$$V^{(s)} = \begin{cases} (1 - s^{-1})^2 & \text{for } \alpha, \beta \geq 1 - s^{-1} \\ W_s(\alpha) & \text{for } \alpha \leq \beta, \ \alpha < 1 - s^{-1} \\ W_s(\beta) & \text{for } \beta \leq \alpha, \ \beta < 1 - s^{-1} \end{cases} \quad (52)$$

Thus if at least one of the two extreme legs has the intrinsic speed less than $1 - s^{-1}$, the speed of the entire spider is solely determined by the slowest leg.

To determine $W_s(\beta)$ we note that velocity on the right boundary is

$$V = \beta(1 - x_{s-1}) = \beta(1 - B\lambda^{s-1}) = \beta\frac{1 - \lambda^{s-1}}{1 - \lambda^s} \quad (53)$$

where in the last step we have used (49). Equating the velocity given by Eq. (53) with the velocity in the bulk given by Eq. (51) we find

$$\beta = \lambda \frac{1 - \lambda^{s-1}}{1 - \lambda^s} \quad (54)$$

Thus the velocity is given by (53) or (51), where parameters are connected via (54).

Explicit results can be obtained for s up to $s = 5$. For $s = 2$ we recover the celebrated result

$$W_2(\beta) = \beta(1 - \beta) \quad (55)$$

For $s = 3$ the final expression is still compact

$$W_3(\beta) = \beta(1 - \beta)\frac{1 + \sqrt{1 + 4b}}{2} \quad (56)$$

with $b = \beta/(1 - \beta)$. For $s = 4$ the result is quite cumbersome

$$W_4(\beta) = \frac{\beta^2}{\lambda}, \quad \lambda = \frac{1}{6}\Delta - \frac{4}{3}\Delta^{-1} - \frac{1}{3} \quad (57)$$

where we have used the shorthand notation

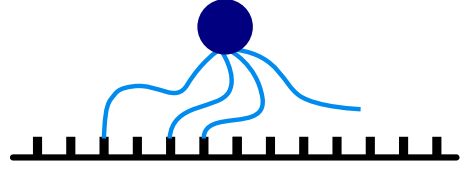$$\Delta = \left\{28 + 108b + 12\sqrt{9 + 42b + 81b^2}\right\}^{1/3}$$

FIG. 2: Illustration of a spider with global constraint. The legs can step independently to nearest neighbor empty sites within a distance S from each other.

B. Global Constraint

For spiders with L legs and maximal span S between any two legs (see Fig. 2), the global constraint rule limits the maximal distance between the extreme legs and the exclusion condition implies that $S \geq L - 1$. A spider with maximal distance $S = L - 1$ is immobile, so we shall tacitly assume that $S \geq L$. It is also useful to keep in mind that for a spider satisfying the local constraint rule the maximal span is $(L - 1)s$ if the maximal distance between the adjacent legs is s; for the bipedal spider $S \equiv s$. A spider with global constraint is equivalent to the exclusion process on a *ring*, where each leg is interpreted as a particle and the total number of sites is equal to $S+1$. For such a process with periodic boundary conditions, a key property of the stationary state, which holds both in symmetric and biased cases, is that all configurations have equal weight [19].

1. Configurations

To count the total number of configurations, we set, as usual, the origin at the position of the extreme left leg, see e.g., (29); this allows us to avoid multiple counting of configurations which differ merely by translation. We then note that the other $L - 1$ legs can occupy sites $1, \ldots, S$. Thus the total number of configurations is

$$\mathcal{C}(L, S) = \binom{S}{L - 1} \quad (58)$$

In the stationary state, the weight of a configuration is thus given by $w = 1/\mathcal{C}$.

Let us now calculate the total number $\mathcal{N}(L, S)$ of $\bullet\circ$ pairs in *all* configurations. Each configuration begins with a string

$$\bullet \underbrace{\circ \cdots \circ}_{a} \bullet \quad (59)$$

where $a = 0, 1, \ldots, S - L + 1$. Disregarding the part up to the second leg maps configurations of the type (59) with fixed a to configurations of the spider with $L - 1$ legs and maximal span $S - a$. The total number of $\bullet\circ$ pairs in these latter configurations is $\mathcal{N}(L - 1, S - a)$. Configurations of the type (59) have of course an additional $\bullet\circ$ pair at

the beginning (when $a > 0$). Therefore

$$\mathcal{N}(L,S) = \sum_{a=0}^{S-L+1} \mathcal{N}(L-1,S-a) + \sum_{a=1}^{S-L+1} \mathcal{C}(L-1,S-a)$$

The latter sum is simplified by using (58) and the identity

$$\sum_{p=q}^{r} \binom{p}{q} = \binom{r+1}{q+1}$$

Thus we arrive at the recurrence

$$\mathcal{N}(L,S) = \sum_{a=0}^{S-L+1} \mathcal{N}(L-1,S-a) + \binom{S-1}{L-2} \qquad (60)$$

The solution (found by a generating function technique or verified by mathematical induction) reads

$$\mathcal{N}(L,S) = L\binom{S-1}{L-1} \qquad (61)$$

Since all configurations have equal weight in the stationary state, the velocity of the biased spider can be expressed by the total number $\mathcal{N}$ of ●○ pairs as

$$V = L^{-1}\frac{\mathcal{N}}{\mathcal{C}}, \qquad (62)$$

which then leads to

$$V = 1 - \frac{L-1}{S} \qquad (63)$$

(Note that the velocity is zero in the unbiased case.) It is more involved to calculate the diffusion coefficient, which we obtain below separately for the unbiased and for the biased case.

2. Symmetric hopping

The diffusion coefficient of the symmetric spider is given by

$$D = L^{-2}\frac{\mathcal{N}}{\mathcal{C}}. \qquad (64)$$

This equation is obtained by applying the fluctuation-dissipation relation, which is valid because the dynamics of the symmetric spider statisfies detailed balance (in other words, the symmetric spider is a system in thermodynamic equilibrium). The Einstein relation then implies that $D \propto V$, where the velocity V of the biased spider is given by the expression (62). The extra factor L^{-1} between (64) and (62) comes from the fact that D is the diffusion coefficient of the left leg (or of the spider's center of mass) whereas V is the mobility of the biased spider where all the legs are asymmetric. Using Eqs. (58) and (61) we recast (64) to

$$D = \frac{1}{L}\left[1 - \frac{L-1}{S}\right] \qquad (65)$$

For the bipedal spider there is no difference between local and global constraints. Using $L = 2$ and $S = s$ we find that Eq. (65) indeed turns into Eq. (3). The calculation of D presented here is self-contained; we notice that the expression (65) can also be found as a special case of a general formula derived in [23] for the diffusion constant of a partially asymmetric exclusion process.

3. Biased hopping

While the velocity (63) is easily computable, the diffusion coefficient was calculated in [24] using a matrix Ansatz (see [19] and [23] for a more general formula). The result is

$$D(L,S) = \frac{1}{2(2S-2L+1)}\binom{2S-1}{2L-1}\binom{S}{L-1}^{-2} \qquad (66)$$

For a given number of legs, the diffusion coefficient of the most clumsy spider is

$$D(L,L) = \frac{1}{2L^2} \qquad (67)$$

while the diffusion coefficient of the most agile spider is

$$D(L,\infty) = \frac{2^{2L-2}}{L}\binom{2L}{L}^{-1} \qquad (68)$$

When $L \gg 1$, the diffusion coefficient (68) scales as

$$D(L,\infty) \sim \frac{1}{4}\sqrt{\frac{\pi}{L}} \qquad (69)$$

More generally, the diffusion coefficient $D(L,S)$ also decreases as $(\pi/16L)^{1/2}$ when $1 \ll L \ll S^{1/2}$.

C. Heterogeneous Spiders

Each leg of a heterogeneous (lame) spider may have its own hopping rate. The bipedal lame spider was studied in Sec. II C. One can find explicit expressions for the velocity and the diffusion coefficient of the lame tripod and perhaps for the lame spider with four legs; the general solution for an arbitrary L is unknown.

Lame spiders are tractable if only one or two legs have different hopping rates. Below we consider lame spiders whose extreme legs are affected. For concreteness, we focus on spiders with local constraint and $s = 2$. The analogy with the TASEP with open boundary conditions still applies, the only modification is that the particle is removed from site 1 with rate α and the particle is added to site $L-1$ with rate β. The flux in such a system was found in Ref. [25]; this gives us

$$V_L(\alpha,\beta) = \frac{C_{L-2}(\alpha,\beta)}{C_{L-1}(\alpha,\beta)} \qquad (70)$$

where we used the shorthand notation

$$C_N(\alpha, \beta) = \sum_{p=1}^{N} \frac{p(2N-1-p)!}{N!(N-p)!} \frac{\alpha^{-p-1} - \beta^{-p-1}}{\alpha^{-1} - \beta^{-1}}$$

Plugging $C_0 = 1$ and $C_1 = \alpha^{-1} + \beta^{-1}$ into (70) we recover the expression (23) for the velocity of the bipedal lame spider; the velocity of the lame tripod is

$$V_3(\alpha, \beta) = \frac{\alpha^{-1} + \beta^{-1}}{\alpha^{-2} + \alpha^{-1}\beta^{-1} + \beta^{-2} + \alpha^{-1} + \beta^{-1}}$$

The speed of the infinite-leg spider exhibits an amusing dependence on the rates α and β:

$$V_\infty = \begin{cases} 1/4 & \text{for } \alpha \geq 1/2, \ \beta \geq 1/2 \\ \alpha(1-\alpha) & \text{for } \alpha \leq \beta, \ \alpha < 1/2 \\ \beta(1-\beta) & \text{for } \beta \leq \alpha, \ \beta < 1/2 \end{cases} \quad (71)$$

Thus if both rates exceed $1/2$, the speed attains a universal (independent of the rates) maximal value $V_\infty = 1/4$. On the other hand, if at least one of the two extreme legs has the intrinsic speed less than $1/2$, the speed of the entire spider is solely determined by the slowest leg.

A general explicit expression for the diffusion coefficient is unknown. There are two special cases, however, in which the diffusion coefficient was explicitly calculated [16]. One is the homogeneous spider ($\alpha = \beta = 1$) when $D(L)$ is given by Eq. (32); another particular case corresponds to $\alpha + \beta = 1$ when the diffusion coefficient is

$$D_L = \frac{1}{2} V_\infty \left\{ 1 - \sum_{k=0}^{L-2} \frac{2(2k)!}{k!(k+1)!} V_\infty^{k+1} \right\} \quad (72)$$

with V_∞ given by Eq. (71); since (72) is valid on the line $\alpha + \beta = 1$, we have $V_\infty = \alpha(1-\alpha) = \beta(1-\beta)$. As a consistency check one can verify that equations (72) and (25) do agree : setting $L = 2$ in the former and $\alpha + \beta = 1$ in the latter we indeed obtain the same result.

The behavior of D_L for the spider with many legs is again amusing. For the infinite-leg spider, Eq. (72) yields

$$D_\infty = \frac{1}{2}\alpha\beta|\alpha - \beta| \quad \text{when} \quad \alpha + \beta = 1 \quad (73)$$

Thus on the line $\alpha + \beta = 1$, the diffusion coefficient vanishes only when $\alpha = \beta = 1/2$.

The behavior of the diffusion coefficient for the infinite-leg spider is particularly neat, and it had actually been understood (in the context of the TASEP) for arbitrary α and β. Derrida, Evans and Mallick [16] found that

$$\frac{D_\infty}{V_\infty} = \begin{cases} 0 & \text{for } \alpha \geq 1/2, \ \beta \geq 1/2 \\ (1-2\alpha)/2 & \text{for } \alpha < \beta, \ \alpha < 1/2 \\ (1-2\beta)/2 & \text{for } \beta < \alpha, \ \beta < 1/2 \\ (1-2\beta)/3 & \text{for } \alpha = \beta < 1/2 \end{cases} \quad (74)$$

The discontinuity on the symmetry line $\alpha = \beta < 1/2$ is especially striking.

IV. QUICK SPIDERS

In the previous sections we have considered the simplest possible gaits when the spider's legs can step only to the neighboring sites. In this section we briefly explore the behavior of quick spiders. These spiders (introduced in Ref. [10]) differ from previously discussed spiders, namely the legs of a quick spider can jump over several lattice sites at once. The only requirement is to stay within distance S from the other legs. Hence quick spiders can be in the same states as the corresponding global spiders, but more transitions are possible between the states of the quick ones.

The simplest quick spider has two legs always next to each other ($L = 2, S = 1$). Although such a global spider cannot move, a quick spider can put one leg ahead of the other and can walk this way. Its motion is completely equivalent to a simple random walk, hence its diffusion coefficient is $D = 1$. This is generally true for quick spiders with L legs and maximal distance $S = L - 1$

$$D(L, S = L - 1) = 1 \quad (75)$$

We also computed the diffusion coefficient of bipedal quick spiders with arbitrary S. We found

$$D(2, S) = \frac{S(S+1)(2S+1)}{6} \quad (76)$$

This expression can be derived using the general formula (64). For the bipedal spider we can label various configuration by the distance $1 \leq \ell \leq S$ between the legs

$$\ldots \circ \bullet \underbrace{\circ \cdots \circ}_{\ell-1} \bullet \circ \ldots \quad (77)$$

Take the left leg. It can jump to the left up to distance $S - \ell$; the corresponding displacements of the center of mass are $\Delta x = -i/2$ with $1 \leq i \leq S - \ell$. The left leg can also jump to the right. The displacements are $\Delta x = i/2$ with $1 \leq i \leq \ell - 1$, and once it overtakes the right leg, $\Delta x = (\ell + i)/2$ with $1 \leq i \leq S$. Taking also into account that all weights are equal, $w_\ell = 1/S$, and recalling that jumping of the right leg will give the same contribution, we recast (64) into

$$D = \frac{1}{4S} \sum_{\ell=1}^{S} \left[\sum_{i=1}^{S-\ell} i^2 + \sum_{i=1}^{\ell-1} i^2 + \sum_{i=1}^{S} (\ell + i)^2 \right] \quad (78)$$

Computing the sum yields the announced result (76).

V. INTERACTING SPIDERS

In experiments [5], thousands of spiders are released, yet their density is usually small. Naively, one can anticipate that spiders are essentially non-interacting. This is correct in the earlier stage, $t < t_*$, but eventually spiders "realize" the presence of other spiders, and their

behavior undergoes a drastic change from diffusive to a sub-diffusive one. This intermediate stage proceeds up to time t^* when spiders explore the entire system and then the diffusive behavior is restored, albeit with a *smaller* diffusion coefficient $\mathcal{D}$. Here we compute $\mathcal{D}$ and estimate the crossover times t_* and t^*.

Let N spiders be placed on the ring of size S. We assume that the spider density $n = N/S$ is low, $n \ll 1$; equivalently the typical distance (n^{-1} lattice spacings) between neighboring spiders is large.

Imagine that we know the diffusion coefficient D of an individual spider (e.g., for the bipedal spider with $s = 3$ we found $D = 1/3$ when each leg hops symmetrically with rates equal to one). Each spider covers around $\sqrt{Dt}$ lattice sites, and equating $\sqrt{Dt_*} = n^{-1}$ we arrive at the estimate of the lower crossover time

$$t_* = \frac{1}{Dn^2} \tag{79}$$

The behavior is sub-diffusive in the intermediate time range, $t_* \ll t \ll t^*$. It is characterized by the $(\lambda t)^{1/4}$ growth of the covered line [26]; this so-called single-file diffusion has numerous applications [27, 28]. The amplitude λ is found by matching $(Dt_*)^{1/2} = (\lambda t_*)^{1/4}$ which in conjunction with (79) yield $\lambda = D/n^2$.

The final behavior is again diffusive. In the long time regime, $t \gg t^*$, we may interpret each spider as an effective particle hopping to the right or left with rates D. The interaction between spiders is essentially equivalent to exclusion interaction between particles, and hence the system reduces to the SEP. We can therefore use (65) where we should replace L by N, and we must also multiply the result by D since spiders effectively hop with rates D rather than one. The term in the brackets in Eq. (65) reduces to $1 - n$; we can replace it by one since $n \ll 1$. Therefore Eq. (65) becomes

$$\mathcal{D} = N^{-1}D \tag{80}$$

Thus exclusion interaction greatly reduces the diffusion coefficient. This strong cooperative effect emerges even when the density is arbitrarily small, the only requirement is that there are many spiders, $N \gg 1$.

The upper crossover time t^* is found by equating $(\mathcal{D}t^*)^{1/2} = (\lambda t^*)^{1/4}$. We arrive at

$$t^* = \frac{S^2}{D} = N^2 t_* \tag{81}$$

Thus the analogy with SEP essentially solves the problem in the practically important limit when the spider concentration is low. Neither memory nor the gait play any role, one must merely use the diffusion coefficient D corresponding to the actual gait and computed under the assumption that the lattice sites are in the product state. One should remember, of course, that the SEP regime is achieved when $t > t^*$; at much earlier times $t > t_*$, the spiders mostly hop on the product, and therefore the assumption of full attachment can become problematic.

VI. DISCUSSION

A single spider is a self-interacting object. There are two sources of interaction between the legs: (i) exclusion (no more than one leg per site), and (ii) legs cannot be too far apart. Is it possible to represent a spider as an effective single particle? The answer is yes — at least in simple situations, one can treat a spider as a diffusing particle. It is far from trivial, of course, to compute the diffusion coefficient of this particle. Fortunately, natural models of spiders are related to simple exclusion processes. In the course of this work we had an advantage of utilizing some beautiful results and powerful techniques developed in the studies of simple exclusion processes.

Our models certainly do not take into account all the details of an experimental situation [5]. For instance, we assumed that the re-attachment of a leg is very quick, so the process is controlled by detachment. Hence spiders remain fully attached and never leave the surface. This assumption is important as our analysis has relied on the permanent presence of spiders on the surface. Relaxing this assumption does not make the problem intractable — indeed in recent analyzes of molecular motors the complete detachment (unbinding) from cytoskeletal filaments is allowed, see e.g. [29, 30, 31, 32, 33]. Further, our analysis of the many-spider situation in Sec. V treats the low density case; the analogy with SEP allowed us to handle the problem but the assumed permanent presence of the spiders is particularly questionable in this case.

Perhaps the most serious limitation of our analysis is the disregard of memory — in experimental realizations [5] spiders often affect the environment which in turn affect their motion. The non-Markovian nature of this problem calls for a set of new techniques even in the case of a single spider. In one dimension, the influence of memory can be probed analytically for a single bipedal spider [8], and the replacement of a self-interacting spider by an effective particle remains valid, though this effective particle becomes an excited random walk which distinguishes visited and unvisited sites.

Finally we note that the SEP and its generalizations occur in various biological problems ranging from motion of molecular motors [29, 30, 31, 32, 33] to protein synthesis [34, 35, 36, 37]. Some models of protein synthesis resemble complicated models of spiders. Another intriguing connection is between spiders and cooperative cargo transport by several molecular motors [38].

APPENDIX A: MASTER EQUATION AND FLUCTUATIONS

In this Appendix, we explain the general formalism, inspired by Ref. [19], that allows one to calculate velocities and diffusion contants, and we use this method to derive equation (28).

A spider can be viewed as a homogeneous Markov process with a finite number of internal states. The dynamics of the spider is encoded in a Markov Matrix M, where the non-diagonal matrix element $M(C, C')$ represents the rate of evolution from a configuration C' to a different configuration C. The quantity $-M(C, C)$ is the exit-rate from configuration C. The master equation for $P_t(C)$, the probability of being in configuration C at time t, is then given by

$$\frac{d}{dt}P_t(C) = \sum_{C'} M(C, C')P_t(C'). \quad (A1)$$

We now define Y_t as the absolute position of the spider's left leg, knowing that at time $t = 0$, $Y_t = 0$. Between t and $t + dt$, Y_t varies by the discrete amount $+1, 0$ or -1 that depends on the configuration C' at t and on the configuration C at $t + dt$. The Markov Matrix M can then be decomposed in three parts corresponding to the three possible evolutions of Y_t :

$$M(C, C') = M_0(C, C') + M_1(C, C') + M_{-1}(C, C'). \quad (A2)$$

For example, $M_1(C, C')$ represents the transition rate from a configuration C' to C with the left leg moving one step forward (this matrix element vanishes otherwise); M_{-1} corresponds to transitions for which the left leg moves one step backwards; M_0 encodes transitions in which the left leg stays still. We call $P_t(C, Y)$ the joint probability of being at time t in the configuration C and having $Y_t = Y$. A master equation, analogous to equation (A1), can be written for $P_t(C, Y)$ as follows :

$$\begin{aligned}\frac{d}{dt}P_t(C, Y) = \sum_{C'} \Big(&M_0(C, C')P_t(C', Y) \\ + &M_1(C, C')P_t(C', Y - 1) \\ + &M_{-1}(C, C')P_t(C', Y + 1)\Big). \quad (A3)\end{aligned}$$

In terms of the generating function $F_t(C)$ defined as

$$F_t(C) = \sum_{Y=-\infty}^{\infty} e^{\lambda Y} P_t(C, Y), \quad (A4)$$

the master equation (A3) takes the simpler form :

$$\frac{d}{dt}F_t(C) = \sum_{C'} M(\lambda; C, C')F_t(C'), \quad (A5)$$

where $M(\lambda; C, C')$, which governs the evolution of $F_t(C)$, is given by

$$M(\lambda) = M_0 + e^{\lambda}M_1 + e^{-\lambda}M_{-1}. \quad (A6)$$

We emphasize that $M(\lambda)$, is not a Markov matrix for $\lambda \neq 0$ (the sum of the elements in a given column does not vanish).

In the long time limit, $t \to \infty$, the behaviour of $F_t(C)$ is dominated by the largest eigenvalue $\mu(\lambda)$ of the matrix $M(\lambda)$. We thus have, when $t \to \infty$,

$$\langle e^{\lambda Y_t} \rangle = \sum_C F_t(C) \sim e^{\mu(\lambda)t}. \quad (A7)$$

This result can be restated more precisely as follows :

$$\lim_{t\to\infty} \frac{1}{t} \log\langle e^{\lambda Y_t} \rangle = \mu(\lambda). \quad (A8)$$

The function $\mu(\lambda)$ contains the complete information about the cumulants of Y_t in the long time limit. For example, the velocity V and the diffusion coefficient D of the spider are given by

$$V = \lim_{t\to\infty} \frac{\langle Y_t \rangle}{t} = \frac{d\mu(\lambda)}{d\lambda}\Big|_{\lambda=0} = \mu'(0), \quad (A9)$$

$$D = \lim_{t\to\infty} \frac{\langle Y_t^2 \rangle - \langle Y_t \rangle^2}{2t} = \frac{\mu''(0)}{2}. \quad (A10)$$

One therefore needs to calculate the function $\mu(\lambda)$. For simple problems such as the bipedal spider with $s = 2$, $\mu(\lambda)$ can be determined explicitly (because $M(\lambda)$ is a 2 by 2 matrix). In general, the most efficient technique is to perform a perturbative calculation of $\mu(\lambda)$ in the vicinity of $\lambda = 0$ (recall that $\mu(\lambda)$ vanishes at $\lambda = 0$). This perturbative approach is very similar to the one used in Quantum Mechanics, the major difference being that $M(\lambda)$ which plays the role of the Hamiltonian is not, in general, a symmetric matrix and its right eigenvectors are different from its left eigenvectors. By definition, we have

$$\begin{aligned}M(\lambda)\,|\,\mu(\lambda)\,\rangle &= \mu(\lambda)\,|\,\mu(\lambda)\,\rangle, \\ \langle\,\mu(\lambda)\,|M(\lambda) &= \mu(\lambda)\langle\,\mu(\lambda)\,|. \quad (A11)\end{aligned}$$

Using equations (A6), (A9), and (A10), we can write the following perturbative expansions in the vicinity of $\lambda = 0$,

$$\begin{aligned}M(\lambda) &= M + \lambda(M_1 - M_{-1}) + \frac{\lambda^2(M_1 + M_{-1})}{2}\cdots \\ \mu(\lambda) &= V\lambda + D\lambda^2 + \dots \\ |\,\mu(\lambda)\,\rangle &= |\,0\,\rangle + \lambda\,|\,1\,\rangle + \lambda^2\,|\,2\,\rangle + \dots, \\ \langle\,\mu(\lambda)\,| &= \langle\,0\,| + \lambda\langle\,1\,| + \lambda^2\langle\,2\,| + \dots\end{aligned}$$

where M is the original Markov matrix of the system, $|\,0\,\rangle$ is the stationary state and $\langle\,0\,| = (1, 1, \dots, 1)$ is the left ground state of M. We now substitute these perturbative expansions in (A11) and identify the terms with the same power of λ. Using the left eigenvector $\langle\,\mu(\lambda)\,|$, we obtain

$$\langle\,0\,|M = 0, \quad (A12)$$

$$\langle\,1\,|M = V\langle\,0\,| - \langle\,0\,|(M_1 - M_{-1}), \quad (A13)$$

$$\begin{aligned}\langle\,2\,|M = D\langle\,0\,| &- \frac{1}{2}\langle\,0\,|(M_1 + M_{-1}) \\ &+ V\langle\,1\,| - \langle\,1\,|(M_1 - M_{-1}). \quad (A14)\end{aligned}$$

Multiplying these equations by the right ground state $|0\rangle$ of M, and using the fact that $M|0\rangle = 0$ and $\langle 0|0\rangle = 1$, the following formulae for V and D are derived as solvability conditions for Eqs. (A12)–(A14) :

$$V = \langle 0|M_1 - M_{-1}|0\rangle, \qquad (A15)$$

$$D = \langle 1|M_1 - M_{-1}|0\rangle$$
$$+ \frac{1}{2}\langle 0|M_1 + M_{-1}|0\rangle - V\langle 1|0\rangle. \quad (A16)$$

We observe that in order to calculate V we only need to know the ground state of M. However, the calculation of D requires the knowledge of $\langle 1|$, obtained by solving the linear equation (A13). We remark that similar expressions can be obtained starting from the expansion of right eigenvector $|\mu(\lambda)\rangle$.

We now specialize this framework to the case of the heterogeneous bipedal lame spider with s internal states. The Markov Matrix is then an $s \times s$ matrix $M = M_0 + M_1$ since M_{-1} vanishes identically. The matrix M_0 is given by

$$M_0 = \begin{pmatrix} -\alpha & & & & & 0 \\ \alpha & -(\alpha+\beta) & & & & \\ & \beta & -(\alpha+\beta) & & & \\ & & \ddots & \ddots & & \\ & & & \beta & -(\alpha+\beta) & \\ 0 & & & & \beta & -\alpha \end{pmatrix}$$

and the matrix M_1 is

$$M_1 = \alpha \begin{pmatrix} 0 & 1 & & & 0 \\ & 0 & 1 & & \\ & & 0 & 1 & \\ & & & \ddots & \ddots \\ & & & & 0 & 1 \\ 0 & & & & & 0 \end{pmatrix}$$

The stationary state of M is $|0\rangle = (p_0, p_1, \ldots, p_{s-1})$ with

$$p_k = \frac{\alpha - \beta}{\alpha^s - \beta^s}\alpha^{s-k-1}\beta^k \quad \text{for} \quad k = 0, \ldots, s-1. \quad (A17)$$

This expression, together with (A15), leads to the formula (27) for the spider velocity.

In order to derive the expression of the diffusion coefficient, we need to solve equation (A13). One can verify that the solution of this equation is given by $\langle 1| = (q_0, q_1, \ldots, q_{s-1})$ where

$$q_k = (k+1)\frac{V-\alpha}{\beta-\alpha} + \frac{\alpha\beta - \alpha V}{(\beta-\alpha)^2}\left(1 - \left(\frac{\alpha}{\beta}\right)^k\right) \quad (A18)$$

for $k = 0, \ldots, s-1$. Inserting equations (A17) and (A18) into the general expression (A16) leads to the formula (28).

We also used the above method to determine the velocity and the diffusion coefficient for centipedes with $s = 3$. The results (Sect. III A 1) were obtained by explicitly constructing the matrices M_0, M_1, and M_{-1}, and performing exact computations using *Maple*. These computations are feasible when the number of legs is sufficiently small. (The total number of configurations is 3^{L-1} for centipedes with $s = 3$, and hence the order of matrices M_0, M_1, M_{-1} quickly grows with L.)

APPENDIX B: GENERALIZED DETAILED BALANCE RELATION

For the symmetric spider, the three matrices M_0, M_1 and M_{-1}, introduced in (A2) to take into account the total displacement of the spider, satisfy the following detailed balance relation

$$M_y(C,C')P^{eq}(C') = M_{-y}(C',C)P^{eq}(C) \qquad (B1)$$

where the equilibrium measure is denoted by P^{eq} and $y = 0, \pm 1$. Equation (B1) implies that the velocity of the spider vanishes. Consider now a spider driven out of equilibrium with a non-vanishing mean velocity. Suppose however, that for the model under consideration there exists a real number ϵ such that the following generalized detailed balance relation is satisfied

$$M_y(\mathcal{C}, \mathcal{C}')P^{eq}(\mathcal{C}') = M_{-y}(\mathcal{C}', \mathcal{C})P^{eq}(\mathcal{C})\exp(\epsilon y), \quad (B2)$$

Here again, P^{eq} is the equilibrium measure corresponding to the symmetric spider. From relation (B2) it is a matter of elementary algebra to prove that the spectra of $M(\lambda)$ and of $M(-\epsilon - \lambda)$ are identical. Therefore

$$\mu(\lambda) = \mu(-\epsilon - \lambda). \qquad (B3)$$

This relation, which is a special case of the general *Fluctuation Theorem* valid for systems far from equilibrium [39, 40, 41], was derived for stochastic systems by Lebowitz and Spohn [42]. Close to equilibrium, when $\epsilon \ll 1$, we can expand equation (B3) for small λ and ϵ. We find at lowest order

$$\mu''(0) = \frac{\mu'(0)}{\epsilon} \quad \text{i.e.,} \quad D = \frac{V}{\epsilon}, \qquad (B4)$$

which is nothing but the classical fluctuation-dissipation relation between diffusion and mobility.

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